

Butyl butyrate
109-21-7 | DTXSID7041702

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.90

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

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Acetamide, N-methyl-N-phenyl-

Measured: 1.51

Predicted: 2.53

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Molinate

Measured: 25.7

Predicted: 14.8

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Butyl ether

Measured: 72.4

Predicted: 32.3

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cis-Nanophine

Measured: 5.01

Predicted: 6.12

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Quinoline

Measured: 3.80

Predicted: 6.66